

ABSTRACT

A maximum-likelihood method for improves an electron density map of an experimental crystal structure. A likelihood of a set of structure factors $\{F_h\}$ is formed for the experimental crystal structure as (1) the likelihood of having obtained an observed set of structure factors $\{F_h^{OBS}\}$ if structure factor set $\{F_h\}$ was correct, and (2) the likelihood that an electron density map resulting from $\{F_h\}$ is consistent with selected prior knowledge about the experimental crystal structure. The set of structure factors $\{F_h\}$ is then adjusted to maximize the likelihood of $\{F_h\}$ for the experimental crystal structure. An improved electron density map is constructed with the maximized structure factors.